DESIGN AND SIMULATION OF CUMENE PLANT USING ASPEN PLUS

A Thesis

By

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Under the esteemed guidance of
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National Institute of Technology Rourkela

CERTIFICATE

This is to certify that the thesis entitled, **"Design and Simulation of Cumene Plant using ASPEN PLUS**" submitted by **Nirlipt Mahapatra** for the requirements for the award of Bachelor of Technology in Chemical Engineering at National Institute of Technology Rourkela, is an authentic work carried out by him under my supervision and guidance.

To the best of my knowledge, the matter embodied in the seminar report has not been submitted to any other University / Institute for the award of any Degree or Diploma.

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ABSTRACT

Cumene production process is gaining importance and so the process needs to be studied and better ideas suggested such that the production cost is reduced. With the advent of computers and simulating software like ASPEN PLUS® it is possible to design and optimize a particular process. Proper design can significantly reduce production cost as well as provide make the process safe and reduce environmental hazards. It has been identified from previous research papers that the cost of materials used is much higher than the cost of energy needed for the process. The materials, unit operations and processes involved are identified. Steady state simulation is done. Each unit is taken into consideration and the variables are optimized. The units are sequentially optimized in the order in which they appear in the rough flow sheet. Use of newer equipments in the process is suggested. The reactor system on being optimised by an equilibrium based approach gave the operating temperature as 360 C and 6:1 Benzene: Propylene ratio in feed. The distillation columns were optimised and the number of trays for benzene column was found to be 20 by 8 and that for cumene column to be 20 by 10. The reflux ratio values were found to be 0.5 and 0.8 respectively for the columns. The optimised temperature for flashing was identified as 92.5 C. The modified flow sheet of the optimised process was prepared which gives the values of all the optimised variables in detail.

Keywords: Simulation, Optimization, Cumene, Benzene, distillation, reactor

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CHAPTER 1

INTRODUCTION

1. INTRODUCTION

1.1 SYSTEM CONSIDERED

The system considered for study, simulation and optimization is a cumene production plant. The process described by Peterson and Schmidt (2002) is taken as base for simulating the system. The process description of Turton et al. (2003) provides relevant and valuable data required for the simulation of the process.

Raw materials fed to the plant are benzene and propylene (may contain propane as an impurity) in which benzene is in excess. Various unit operations and processes are required to be taken care of which are described in some detail below. The major units in the process plant are the reactor section and the separator section.

1.2 RELEVANCE

Isopropyl benzene popularly known as cumene is the principal chemical used in the production of phenol and its co-product acetone on an industrial scale. It is also the starting material in the production of acetophenone, methyl styrene, diisopropyl benzene and dicumyl peroxide. Minor uses of cumene include as a thinner for paints, enamels, and lacquers; as a constituent of some petroleum-based solvents, such as naphtha; in gasoline blending diesel fuel, and high-octane aviation fuel. It is also a good solvent for fats and resins and has been suggested as a replacement for benzene in many of its industrial applications.

Around 98% of cumene is used to produce phenol and its co-product acetone. However, the requirement of cumene is largely dependent on the use of phenol's derivatives which have resulted in increasing requirement rates for cumene. The largest phenol derivative is bisphenol-A (BPA) which supplies the polycarbonate (PC) sector. PC resins are consumed in automotive applications in place of traditional materials such as glass and metals. Glazing and sheet uses, such as architectural, security and glazing outlets, are also important PC applications. The third largest use for PC is optical media such as compact discs (CDs) and digital versatile discs (DVDs). Another phenol derivative is caprolactam which is used mainly to make nylon 6. It is mainly the resin sector of the nylon market that is seeing growth. [Schmidt, 2005]

Cumene is produced by the alkylation of benzene with propylene over an acid catalyst like aluminium chloride, boron trifluoride, phosphoric acid, hydrogen fluoride, supported phosphoric acid (SPA) etc. The usage of the above catalysts poses a lot of problems like product quality, lower catalyst activity, environmental hazard, catalyst non-regenerability etc and has been replaced by zeolites in most of the processes.

In the present work the cumene production plant is simulated using ASPEN PLUS ® and the sizes, the temperature and other relevant parameters are obtained by optimization. MATLAB®, MS Excel and Origin Pro 8.0 are used to plot graphs in the following simulation from which an optimum value is estimated. The optimized values obtained can provide a lot of insight before actual plant commissioning is done.

1.3 OBJECTIVE OF THE PROJECT

Considering the importance of the present process, work was undertaken to design and simulate the cumene production process using ASPEN PLUS ® software. The objectives of the present project are following.

- To design a zeolite catalyst based cumene production process and study the sensitivity analysis.
- To optimize the contents of the flow sheet for minimization of loss of material along with a greater production of cumene and low requirement of energy.

CHAPTER 2

LITERATURE REVIEW

2. LITERATURE REVIEW

2.1 CONVENTIONAL PROCESS

Cumene is produced by the alkylation of benzene with propylene over an acid catalyst. Catalysts like aluminium chloride, boron trifluoride, hydrogen fluoride and solid phosphoric acid (SPA) are normally used. Over the years these catalysts have given way to zeolite based catalysts. There are some inherent problems associated with the conventional acid catalysts.

Disadvantages of using solid phosphoric acid (SPA) Process

1. Lower activity
2. Catalyst non-regenerability
3. Unloading of spent catalyst from reactor difficult
4. Relative high selectivity to hexyl benzene
5. Significant yield of DIPB

Disadvantages of using Aluminium chloride as catalyst

1. High corrosion
2. Environmental hazard
3. Washing step for catalyst removal.

2.2 CURRENT INDUSTRIAL PROCESS

Cumene is an important chemical in the present industrial world and its uses are steadily increasing. The process followed for the production of cumene is the catalytic alkylation of benzene with propylene and now a days zeolite based catalysts are used in place of the normal acid based catalysts due to added advantages. Cumene production process has been greatly studied and the reaction mechanism and the reaction kinetics have been specified by many researchers. Both experimental as well as computer based simulation and optimization studies have been carried out by various researchers. The significant works of various researchers which have been helpful in my project are described in brief below.

The Q-Max ™ process converts a mixture of benzene and propylene to high quality cumene using a regenerable zeolite catalyst. The Q-Max ™ process is characterized by a exceptionally high yield, better product quality, less solid waste, decrease in investment and operating costs and a corrosion free environment. The Q-Max ™ process developed by UOP uses QZ-2000/ QZ-2001 catalyst which is a variant of β - zeolite. [Schmidt, 2005]

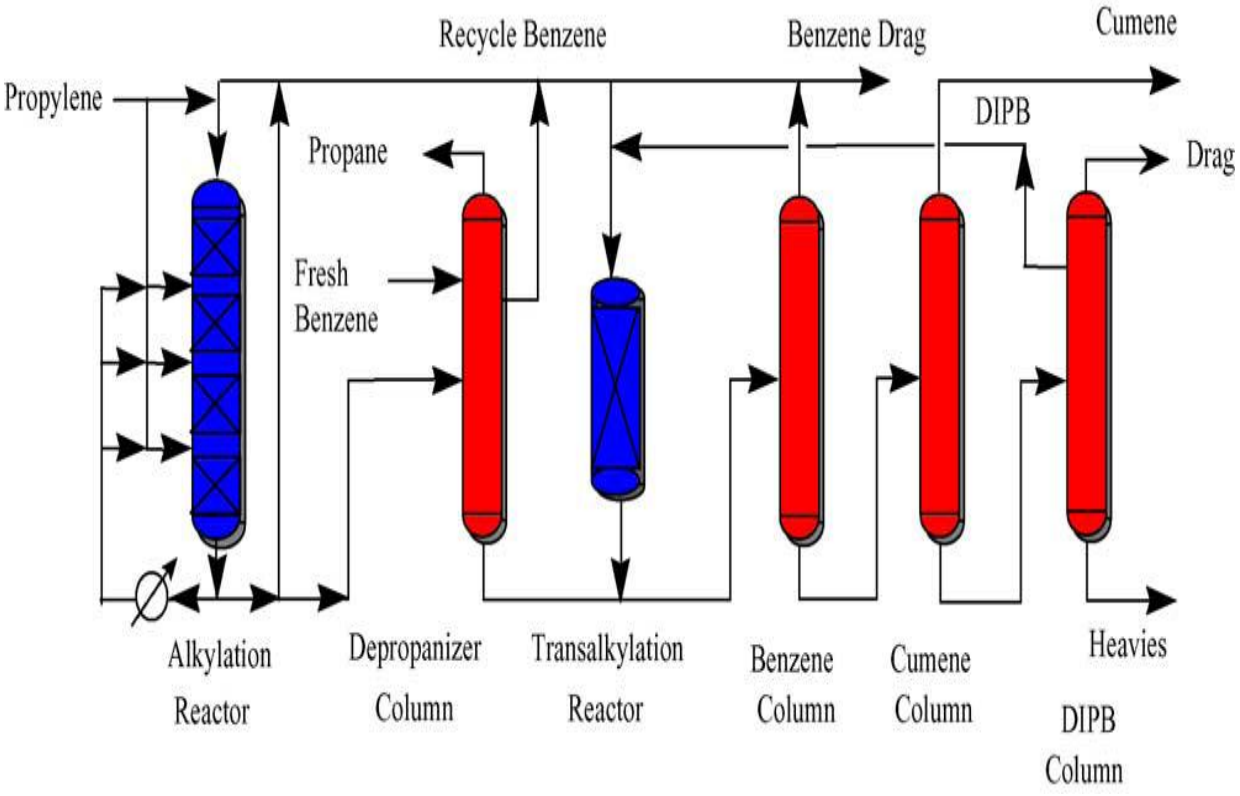


Fig. 2.1 Q-Max process flow diagram [Schmidt, 2005]

2.2.1 PROCESS DESCRIPTION

The Q-MAX™ process provides a very good cumene yield and quality. The QZ-2000 zeolite based catalyst used in the Q-MAX™ process operates with a low flow rate of benzene and hence investment and utility costs are reduced greatly. QZ-2000 is non-corrosive and regenerable, avoiding the significant maintenance and catalyst disposal problems associated with SPA and $AlCl_3$ systems. Compared to other zeolite based cumene technologies, the Q-MAX™ process provides the highest product quality and great stability. Impurities in the feed have less effect.

The Q-MAX™ process flow scheme is shown in fig 2.1 above. The alkylation reactor is divided into four catalytic beds present in a single reactor shell. The fresh benzene feed is passed through the upper-mid section of the depropanizer column to remove excess water and then sent to the alkylation reactor. The recycle benzene to the alkylation and transalkylation reactors is drawn from the benzene column. This mixture of fresh and recycle benzene is charged through the alkylation reactor. The fresh propylene feed is split between the catalyst beds and is fully consumed in each bed. An excess of benzene helps in avoiding poly alkylation and minimizing olefin oligomerization. Because the reaction is exothermic in nature, the temperature rise in the alkylation reactor is controlled by recycling a portion of the reactor effluent to the reactor inlet to act as a heat sink. The inlet temperature of each downstream bed is further reduced to the same temperature as the first bed inlet by injecting a portion of cooled reactor effluent between the beds. Effluent from the alkylation reactor flows to the depropanizer column which removes the propane the excess water. The bottoms stream of the depropanizer column goes to the benzene column where excess benzene is collected overhead and recycled. The benzene column bottoms stream goes to the cumene column where cumene is recovered overhead. The cumene column bottoms stream, predominantly diisopropylbenzene (DIPB), goes to the DIPB column. If the propylene feed contains excessive butylenes, or if the benzene feed contains excessive toluene, butylbenzenes and/or cumene are distilled out and purged from the overhead section of the DIPB column. The DIPB stream leaves the column by way of the side draw and is recycled back to the transalkylation reactor. The DIPB column bottoms consist of heavy aromatic by-products, which are normally blended into fuel oil. Steam or hot oil provides the heat for the product fractionation section. The recycle DIPB from the overhead of the DIPB column combines with a portion of the recycle benzene and is charged downflow through the transalkylation reactor. In the transalkylation reactor, DIPB and benzene are converted to more cumene. The effluent from the transalkylation reactor is then sent to the benzene column. The new QZ-2001 catalyst is utilized in the alkylation reactor while the original QZ-2000 catalyst remains in the transalkylation reactor. Expected catalyst cycle length is 2–4 years, and the catalyst should last for at least three cycles with proper care. At the end of each cycle, the catalyst is typically regenerated ex situ via a simple carbon burn by a certified regeneration contractor. However, the unit can also be designed for in situ regeneration. The Q-Max™ process typically produces near equilibrium levels of cumene (between 85 and 95 mol %) and DIPB (between 5 and 15 mol %). The DIPB is separated from the cumene and is reacted with

recycle benzene at optimal conditions for transalkylation to produce additional cumene. [Schmidt, 2005], [Peterson and Schmidt, 2002]

2.2.2 REACTION MECHANISM AND KINETICS

The following reaction mechanisms are proposed for the alkylation of benzene to cumene process. The major reactions taking place are *alkylation* and *trans-alkylation*. The other reactions involved include *isomerisation* and *dis-proportionation*. The reaction mechanism as well as the reaction kinetics may vary depending on the catalyst used. The reaction can proceed by with or without carbonium ion intermediate. [Ding and Fu, 2005]

The rates of reaction data was obtained for different catalysts from the work done by various researchers. The kinetic data and the reaction conditions specified by Turton et al (2003) for a particular catalyst have been used in the present work.

The reaction kinetic data is shown below

Propylene + benzene → cumene

K = 2.8×10^7

E (kJ/kmol) 104174

Rate=kc_pc_b

Propylene + cumene → p-diisoproyl benzene

K = 2.32×10^9

E (kJ/kmol) 146742

Rate=kc_pc_c

(The unit for rates is kmol s^{-1} m^{-3})

[Turton et al, 2003]

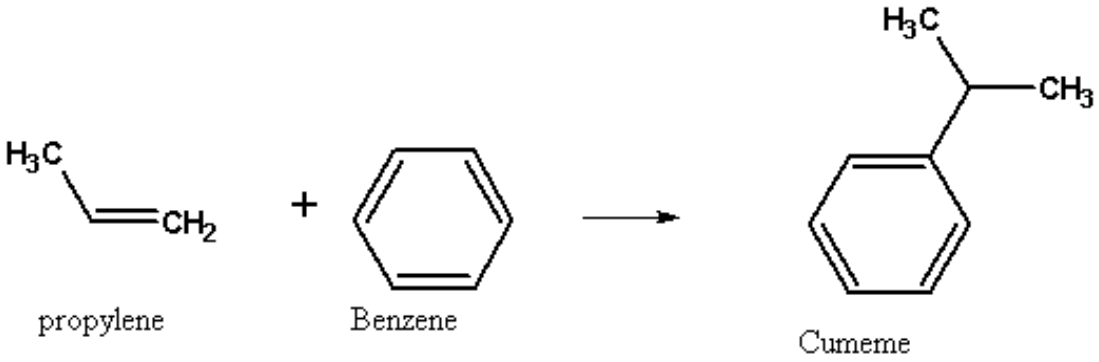
Trans-alkylation reaction

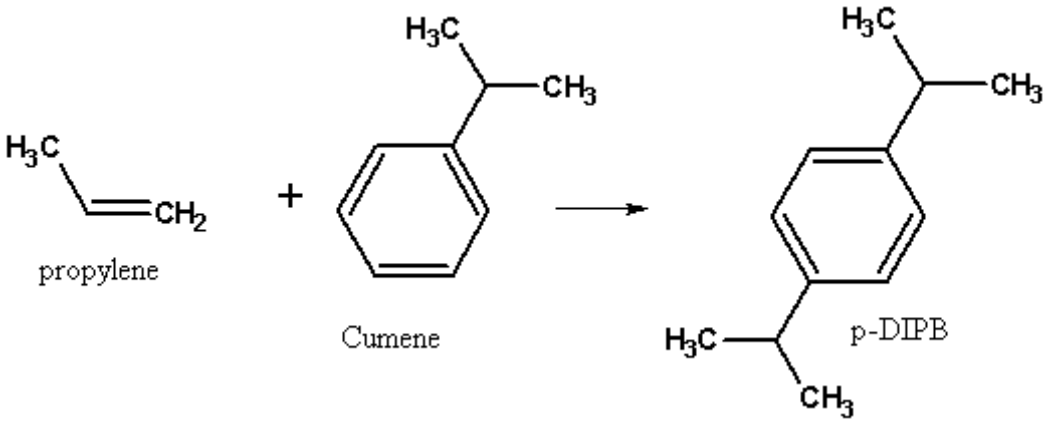
K= 6.52×10^{-3} exp (27240/RT)

The equilibrium data for trans-alkylation reaction is obtained for modified zeolite beta catalyst, YSBH-01. [Lei et al, 2007]

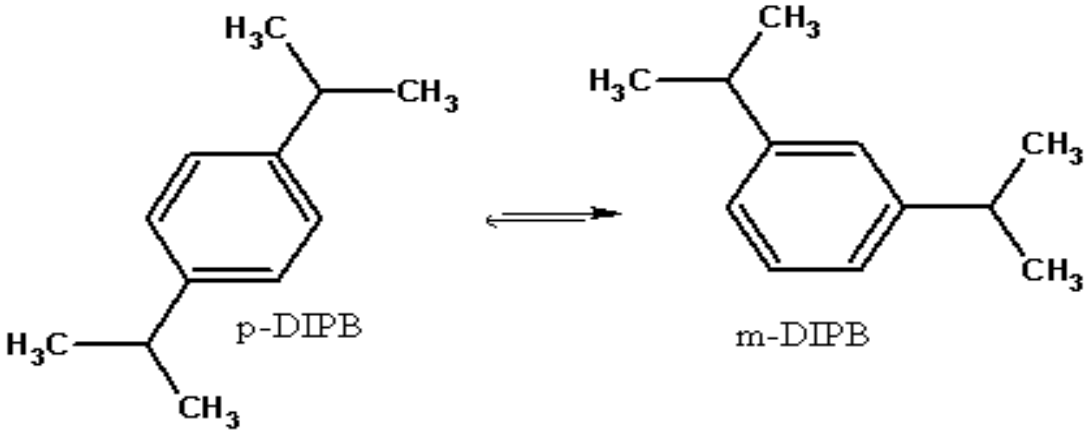
From various works on cumene production mechanism the overall reaction can be assumed to consist of the following stages.

Alkylation

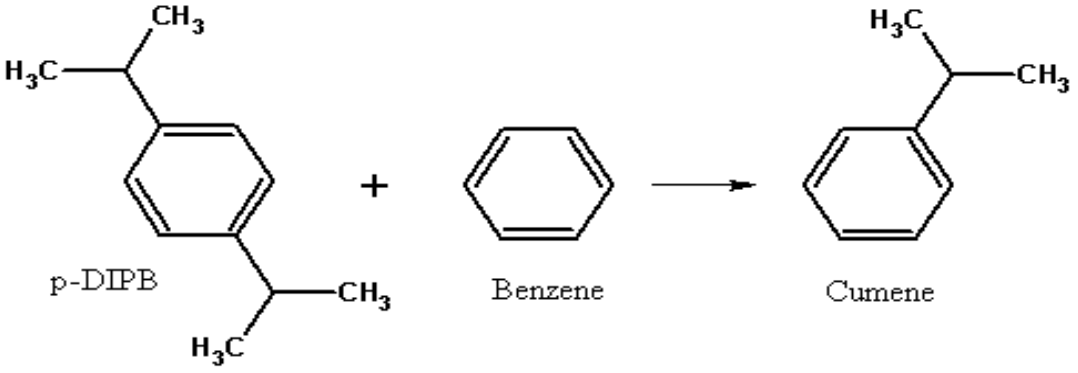


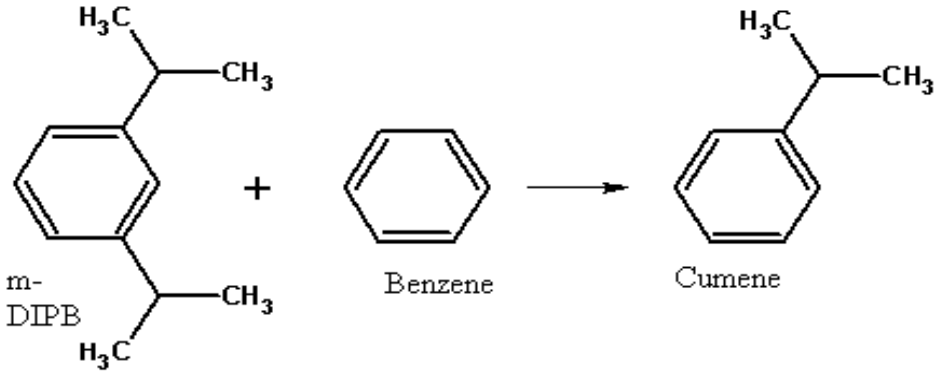


Isomerisation

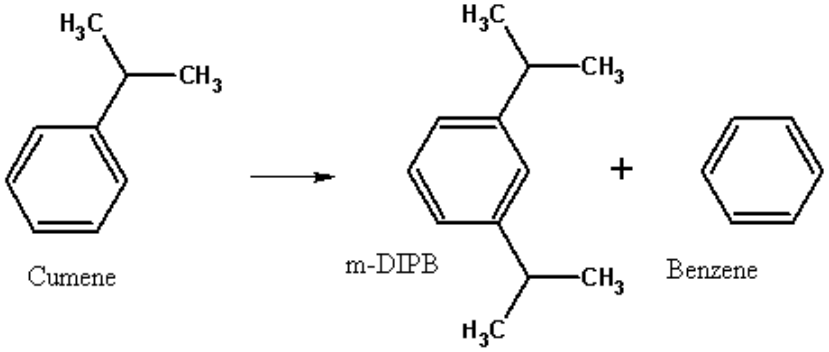


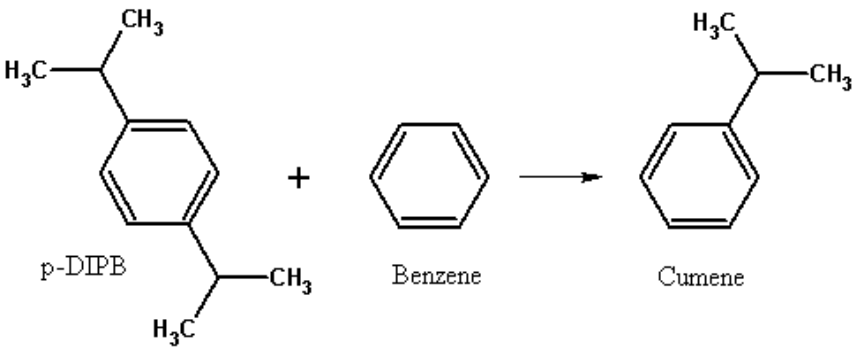
Transalkylation





Dis-proportionation





2.3 PROPERTIES OF CUMENE

- *Description*: Colorless liquid with a sharp, penetrating aromatic or gas-like odour [Budavari, 1989; Cavender, 1994]
- *Boiling Point*: 152.4°C [Lide, 1995]
- *Melting Point*: -96.0°C [Lide, 1995]
- *Density*: 0.8618 g/cm^3 at 20°C [Lide, 1995]
- *Refractive Index*: 1.4915 at 20°C [Schulz *et al*., 1993]; 1.489 at 25°C [Lewis, 1993]
- *Solubility*: Insoluble in water; miscible in acetone, benzene, and ethanol [Lide, 1995]
- *Flash Point*: 39°C, closed cup [Budavari, 1989]
- *Reactivity*: Combustible [Lewis, 1993], not compatible with oxidizers, nitric acid and sulphuric acid.

2.4 PROCESS DESIGN BASICS

Process design is a very important aspect before any project implementation as a proper design during the initial stages can save costs to a great extent. The cost involved in designing a project is very less compared to the construction cost and it can be greatly helpful in maximizing profits of the plant as well as providing a safe environment. The plot shown in Fig. 2.2 gives a brief idea of how proper plant design can cut costs to a great extent.

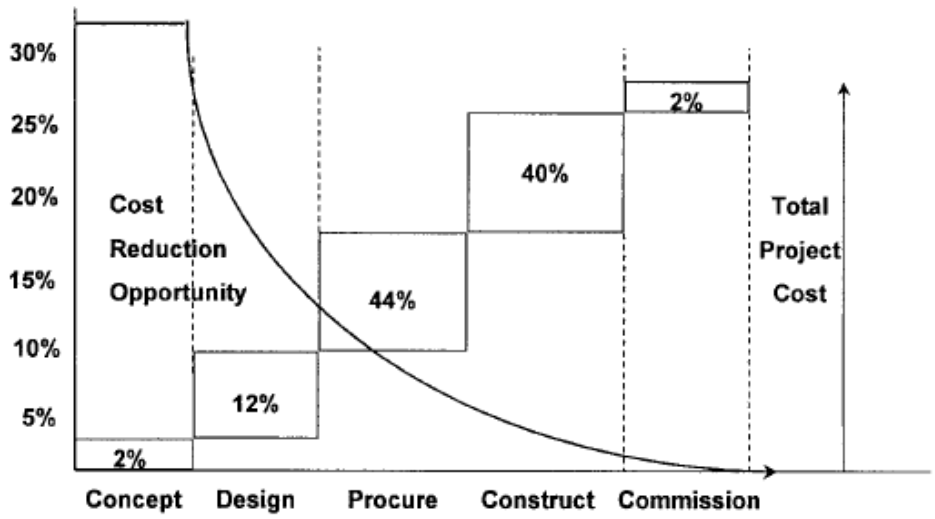


Fig 2.2 Cost reduction during project implementation [Dimian, 2003]

The following points need to be taken care for a proper process design.

1. *Raw material cost reduction*. Selectivity of reaction is increased by proper use of catalysts. Increasing selectivity can reduce separation and recycle costs.
2. *Capital-cost reduction*. Better flow sheeting can reduce capital costs effectively
3. *Energy use reduction*. Pinch point analysis is used for energy saving.
4. *Increased process flexibility*. Process plant should be able to handle a range of feed compositions.
5. *Increased process safety*. Nonlinear analysis can be done to make the process safer.
6. *Increased attention to quality*. Reduction of by products and the effective use of process control equipment can lead to process safety.
7. *Better environmental performance.* Minimization of harmful wastes to the environment.

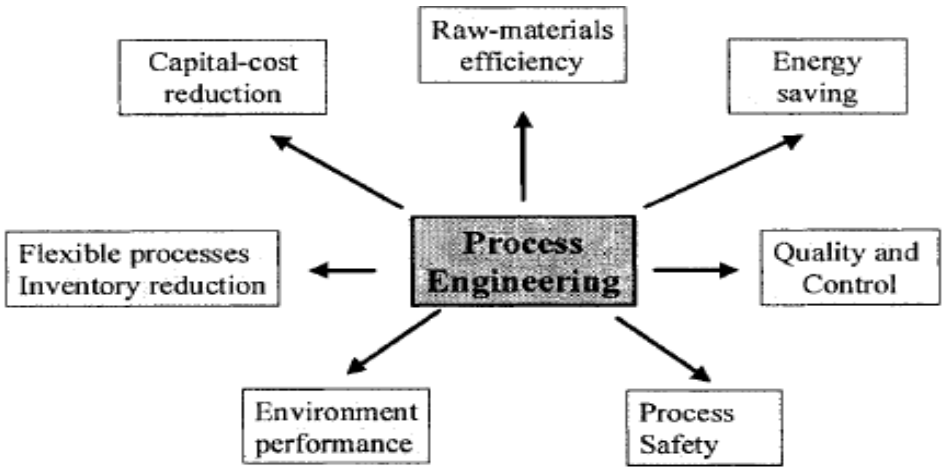


Fig 2.3 Factors to be considerd during process design [Dimian, 2003]

The order in which designing should be done follows a systematic procedure as shown in Fig 2.4.

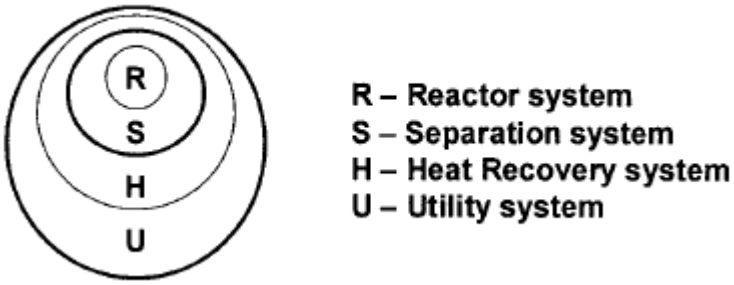


Fig 2.4 Onion Diagram (traditional process design hierarchy of phases) [Linnhoff, 1994]

A process simulation diagram is drawn from the process flow diagram. The chemical components are specified. The chemical component properties are generally available in a standard data base. The input streams are specified. Thermodynamic modelling is done. Series of simulations are run for convergence of a particular variable. Sensitivity analysis which consists of varying the sampled variables as a function of the manipulated variables is normally done. The major parts of a cumene production plant are reactor system, separation system and they are optimized.

CHAPTER 3

DESIGN: PROCEDURE, RESULT & DISCUSSION

3. DESIGN: PROCEDURE, RESULT AND DISCUSSION

3.1. SEQUENCE OF COMPUTATION

This chapter is divided into two main parts as (i) Reactor and (ii) Separator. The reactor design involves design of equilibrium based reactor as well as kinetic based reactor. The separator system involves the design of flash tank and distillation column. As the product purity is increased by increasing the working cost of the reactor, the separation cost decreases and vice versa. The sequence of computation followed is shown in Fig. 3.1.

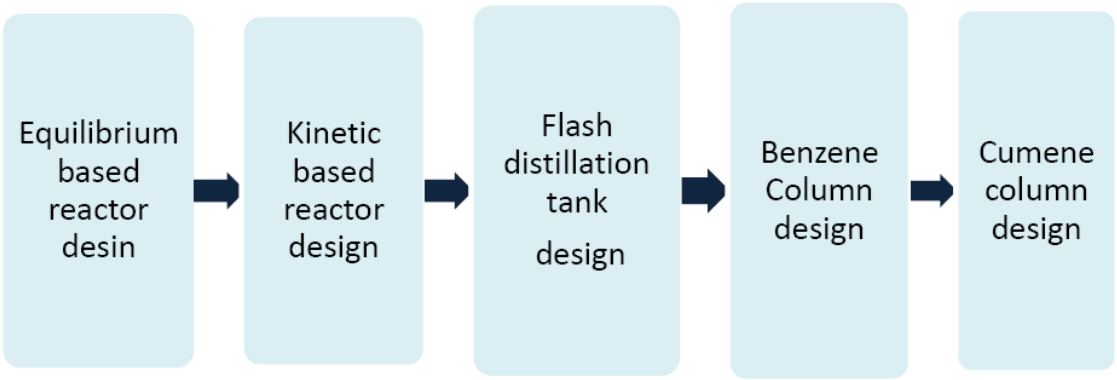


Fig 3.1 Sequence of computation

3.2 REACTOR DESIGN

Reactor is the heart of a chemical process plant. Design of a reactor requires data from thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer and economics. A properly designed reactor can minimize the production of unwanted products and hence reduce the purification costs.

The *alkylation* and *trans-alkylation* reactors are the main reactors in a cumene production plant and they need to be designed for optimum use of material and energy. In all the optimization work done *Douglas Doctrine* (the costs of raw materials and products are usually much larger than the costs of energy or capital in a typical chemical process. Therefore the process must be designed (investing capital and paying for energy) so as to not waste feed stocks or lose products (particularly in the form of undesirable products) is

followed. [Luyben, 2010] Kinetic model can be considered if accurate kinetic data is available. But a plant involves industrial reactors that are very complex and hence a proper combination of stoichiometric and kinetic reactor needs to be used. Kinetic model can determine the production rate where as stoichiometric model can describe the formation of by products and impurities necessary for the design of separators. Equilbrium based reactors like RGIBBS in ASPEN PLUS® can give a realistic idea about the maximum achievable performance. They work accurately for fast reactions. The RGIBBS reactor predicts the equilibrium concentration by Gibbs free energy minimization. [Dimian, 2003] Generally in reactor design an equilibrium model is prepared and then the kinetic model.

The following reaction mechanism was proposed by various researchers for alkylation of benzene by cumene.

3.2.1 REACTIONS CONSIDERED FOR MODELING

Alkylation

propylene + benzene → cumene (1)

propylene + cumene → *p*-diisoproyl benzene (2)

Isomerisation

p-diisopropyl benzene → *m*-diisopropyl benzene (3)

Trans-alkylation

p-diisopropyl benzene + benzene → 2 cumene (4)

m-diisopropyl benzene + benzene → 2 cumene (5)

Disproportination

2 cumene → *p*-diisopropyl benzene + benzene (6)

2 cumene → *m*-diisopropyl benzene + benzene (7)

3.2.2 REACTOR DESIGN PROCEDURE IN ASPEN PLUS

The feed is a mixture of benzene and propylene such that benzene is in excess. In general propylene is not available in the pure form and has some amount of propane as inert. The separation cost of propane is high and hence normally propane is not removed from the propylene feed into the reactor. A high conversion of propylene is desired and the unreacted

propylene can be flashed off along with the inert propane. RGIBBS reactor works by Gibbs free energy minimization. Alkylation and trans-alkylation reactors need not be modelled separately as they can be combined into one equilibrium reactor. The reactant, products as well as the intermediates as seen from the reaction mechanisms are specified into the component list. SYSOP0 or Ideal property table is used. A temperature range of 300 to 400 degree Celsius is specified and a proper temperature chosen. Pressure of 25 atm is chosen from previous industrial research work. [Luyben, 2010]

3.2.3 EQUILIBRIUM STUDIES

The equilibrium is affected by the temperature as well as the benzene/propylene mole ratio. The alkylation and transalkylation reaction is usually carried out at atmospheric pressure. Therefore, the effect of pressure on the equilibrium was not considered in the present study.

Seven reactor models are available in ASPEN PLUS. The equilibrium based RGIBBS reactor is used to find the product composition at which the Gibbs free energy of the product is minimum. The restricted chemical equilibrium approach is used and the reactions mentioned above are specified. The temperature approach for an individual reaction is used. The feed stream mole flow is set as 1 kmol / hr and the feed stream consists of benzene, propylene and propane (inert mixed with the propylene stream). Amount of inert in feed is kept fixed. The reactor temperature is set to 350^0C and the reactor pressure is set to 25 atm. (a) The selectivity of cumene and conversion of propylene (limiting reagent) is studied by varying the benzene/propylene mole ratio in the feed keeping the amount of inert fixed. The effect of temperature variation (300–400^0C) on the selectivity and the conversion is also studied. (b) Again, the variation in the selectivity of *m*-DIPB and *p*-DIPB with temperature and benzene/propylene mole ratio in the feed is studied. The conversion and selectivity were calculated using equations 8 to 11.

$$\%\text{Selectivity of cumene} = F_{\text{cumeneproduct}} / (F_{\text{propylenefeed}} - F_{\text{propyleneprod}}) \times 100\% \quad (8)$$

$$\%\text{Conversion of propylene} = (F_{\text{propylenefeed}} - F_{\text{propyleneprod}}) / F_{\text{propylenefeed}} \times 100\ \% \quad (9)$$

$$\%\text{Selectivity of } m\text{-DIPB} = F_{\text{mdipbproduct}} / (F_{\text{propylenefeed}} - F_{\text{propyleneprod}}) \times 100\% \quad (10)$$

$$\%\text{Selectivity of } p\text{-DIPB} = F_{pdipbproduct}/(F_{propylenefeed}-F_{propyleneprod}) \times 100\% \quad (11)$$

Where

$F_{cumeneproduct}$ = molar flow rate of cumene in product

$F_{propylenefeed}$ = molar flow rate of propylene in feed

$F_{propyleneprod}$ = molar flow rate of propylene in product

$F_{mdipbproduct}$ = molar flow rate of *m*-DIPB in product

$F_{pdipbproduct}$ = molar flow rate of *p*-DIPB in product

RSTOIC reactor model was used to find the standard heat of reaction for different reactions 1 to 6 mentioned above. The standard heats of reaction have been tabulated in Table 3.1. The heat of reaction for isomerisation was found to be zero as expected. The all other reactions were found to be exothermic except trans-alkylation reactions as observed from the table.

Table 3.1 Standard Heats of Reaction

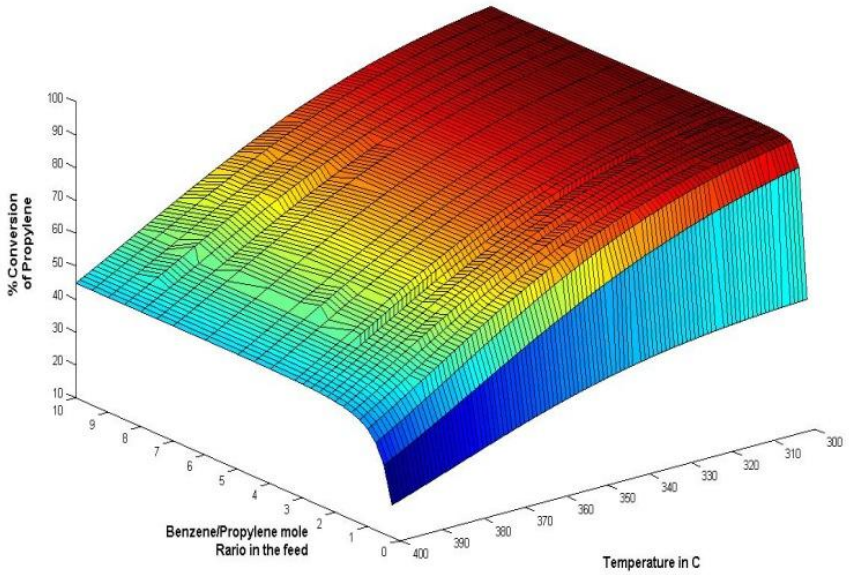
Reaction Number	Standard Heat of Reaction (Kcal/Kg mol)
1	-23.670
2	-24.321
3	0
4	0.649
5	0.649
6	-0.325
7	-0.324

Effect of temperature and benzene/propylene mole ratio.

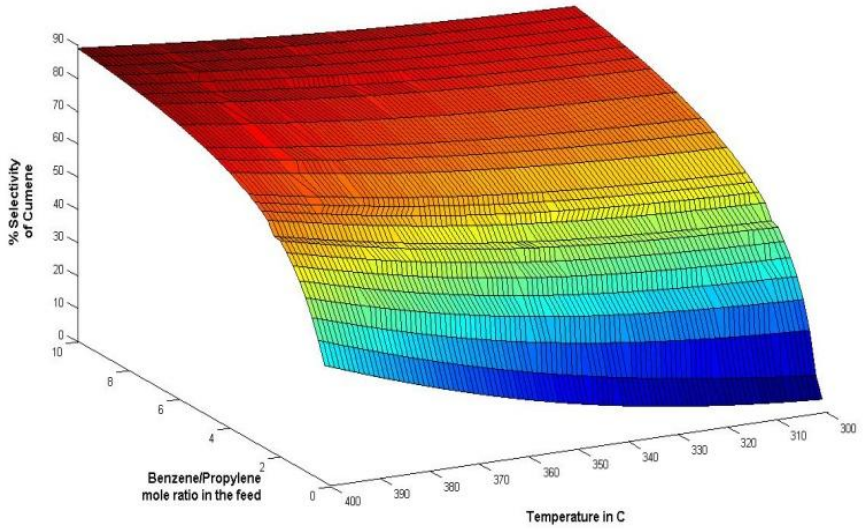
The effect of temperature and benzene/propylene mole ratio on equilibrium conversion of propylene and selectivity of products, cumene, m-DIPB, and p-DIPB is shown in Fig. 3.2. The conversion of propylene was found to increase with increase in benzene/propylene mole ratio for a fixed temperature as observed from the Fig. 3.2(a). This is because of reduced proportion of propylene in feed. However, variation of conversion of propylene was found to be negligibly small above the benzene/propylene mole ratio in feed of 3. The conversion of propylene was found to decrease with increase in temperature for a fixed benzene/propylene

mole ratio as observed from the Fig. 3.2(a). This is because of the fact that overall heat of reactions is exothermic as shown in Table 3.1.

The selectivity of cumene was found to increase with increase in benzene/propylene mole ratio at a fixed temperature as the polyalkylation reactions are reduced because of excess amount of benzene present in the feed (Fig. 3.2(b)). Again, with increase in temperature, the selectivity of cumene increases for a fixed benzene/propylene mole ratio as transalkylation reactions (endothermic, Table 3.1) are dominant at high temperature.



(a)



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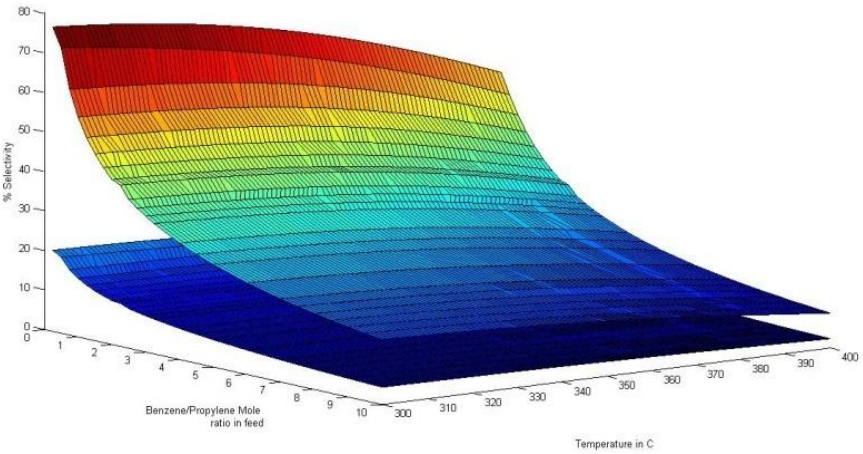
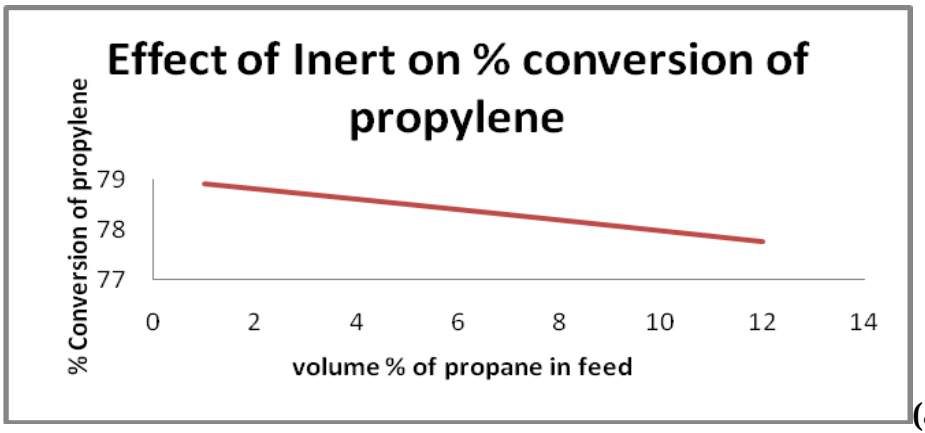
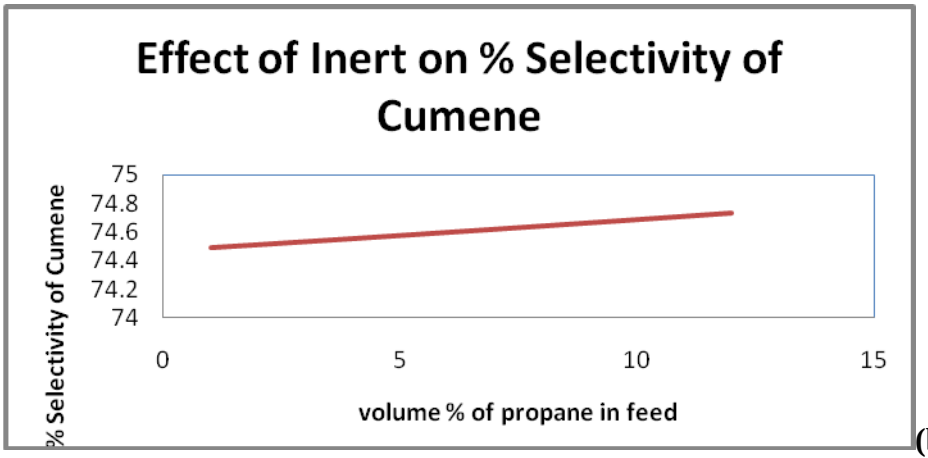


(c)

Fig 3.2 Effect of temperature and benzene/propylene mole ratio on equilibrium (a) conversion of propylene, (b) selectivity of cumene, and (c) selectivity of *m*-DIPB and *p*-DIPB.



(a)



(b)

Fig. 3.3 Effect of inert on equilibrium (a) conversion of propylene (b) selectivity of cumene

The distribution of *m*-DIPB and *p*-DIPB is shown in Fig. 3.2 (c). From the figure it was observed that selectivity of *m*-DIPB is significantly higher than *p*-DIPB. This is because of the fact that *m*-DIPB is thermally more stable compared to *p*-DIPB. Therefore, *p*-DIPB formed in alkylation reaction isomerises to more stable meta isomer.

Effect of inert on equilibrium. The propylene stream used in alkylation process is usually obtained by pyrolysis of petroleum fractions that contains small amount of propane as impurity. Propane need not be removed from the propylene stream as it acts as an inert and does not take part in the reaction. Presence of inert has very slight effect on the conversion as well as selectivity as shown in Fig.3.3. The conversion of propylene decreases slightly with higher volume percent of inert in feed and increases slightly with the same.

3.2.4 KINETICS BASED REACTOR MODEL

Kinetics based rate data was obtained from the work of various researches and is mentioned above. A RPLUG model is used in ASPEN PLUS to model the reactor. The design model specified in the book by Turton et al (2003) is used. The reactions occur in the vapour phase in the presence of a solid catalyst (assumed to have 0.5 void fraction and a 2000 kg/m3 solid density). The reactor is run at high pressure (25 bar) since the moles of reactants are more than the moles of product (Le Chatelier's principle). A temperature of 360 degree C and a benzene/Propylene mole ratio of 6 is used. A flow rate of 330 kmol/hr is used for the simulation.

The kinetic model generated few errors such as RPLUG exited because integration failed. index = (-1) probable cause is incorrect kinetics. check rate-constant parameters and molar volume calculations.

3.2.5 PRODUCT OUTPUT FROM REACTOR

Assuming the RGIBBS model for the initial calculations for distillation columns can give a good idea about the distillation process in a cumene plant. RGIBBS model with an input feed rate of 100 kmol/hr and benzene: propylene feed ratio of 6:1 with an inert concentration of 5% in propylene stream, temp. of 360 degree C and a pressure of 25 bar is used. The flow

rates obtained at the product side are noted.The non condensable components in the product side i.e. propylene and propane are removed in flash tank. These components have fuel value only as they cannot be completely purified. So the reaction conditions should be so adjusted that the propylene in feed is totally converted to the product. The concentration of non-condensable components from reactor is given in Table 3.2. This data is used for further designing.

Table 3.2 Mole flow rate of components from reactor

Component	Mole Flow kmol/hr
Benzene	72.85
Cumene	10.31
m-DIPB	1.77
p-DIPB	0.47
TOTAL	85.4

3.3 PREDICTING VLE CHARACTERISTICS

Reactors and separators can be considered as the back bone of any chemical process plant. The cost optimization of any plant depends largely on the reactors and the distillation columns. The basis of distillation is phase equilibrium that may be VLE (Vapour liquid equilibrium) and LLE (Liquid liquid equilibrium). Before designing any distillation equipment the VLE characteristics need to be studied as they give a fair amount of idea about the ease of distillation. The Txy diagram or temperature versus liquid composition (x) and vapour composition (y) are plotted. A fat curve generally shows that the liquids in a mixture can be easily separated.

The boiling point data of the three major components in the distillation column is shown in Table 3.3 below.

Table 3.3 Boiling point of components

Component	Boiling point in degree Celsius
Benzene	80.2
Cumene	152.4
DIPB	209.8

The product stream from a condenser tank is sent to a distillation column. RADFRAC model is used. In the industrial process three distillation columns are used i.e benzene column, followed by cumene column and DIPB column.The RADFRAC model is a rigorous model for various multistage liquid vapour fractionation operations and hence is used for the simulation Before going in for the design of the distillation column the VLE diagrams need to be considered. The industrial processes currently followed show that in the 1st column benzene and cumene need to be primarily separated and in the 2nd column cumene and DIPB need to be separated. The NRTL (non random two liquid) physical property package is used used to plot the vapour liquid equilibrium T-XY for Benzene-cumene and Cumene-DIPB systems. The VLE plots are shown in Fig 3.4 to 3.6 for different systems.

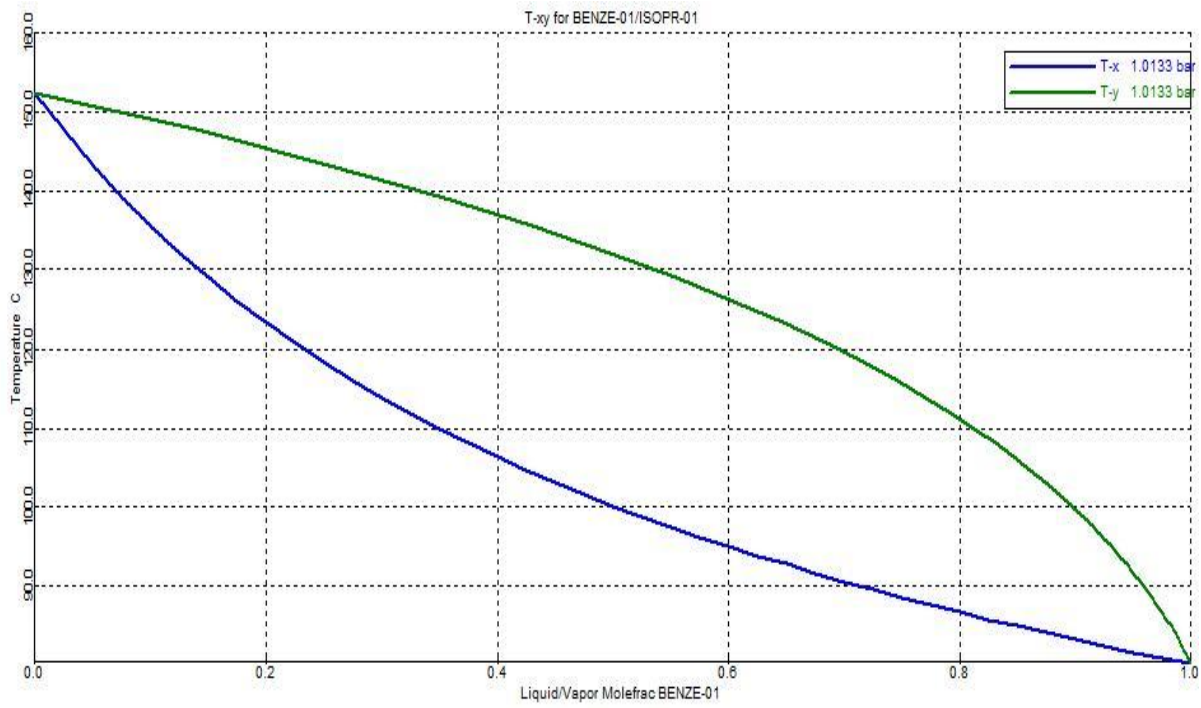


Fig 3.4 Txy for benzene - cumene system

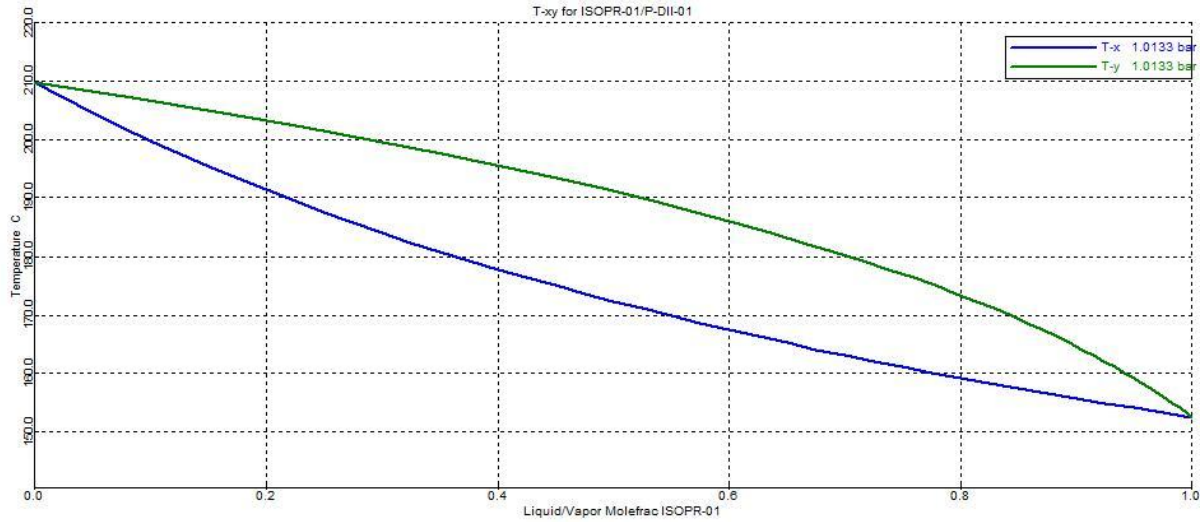


Fig 3.5 Txy for cumene-p-DIPB system

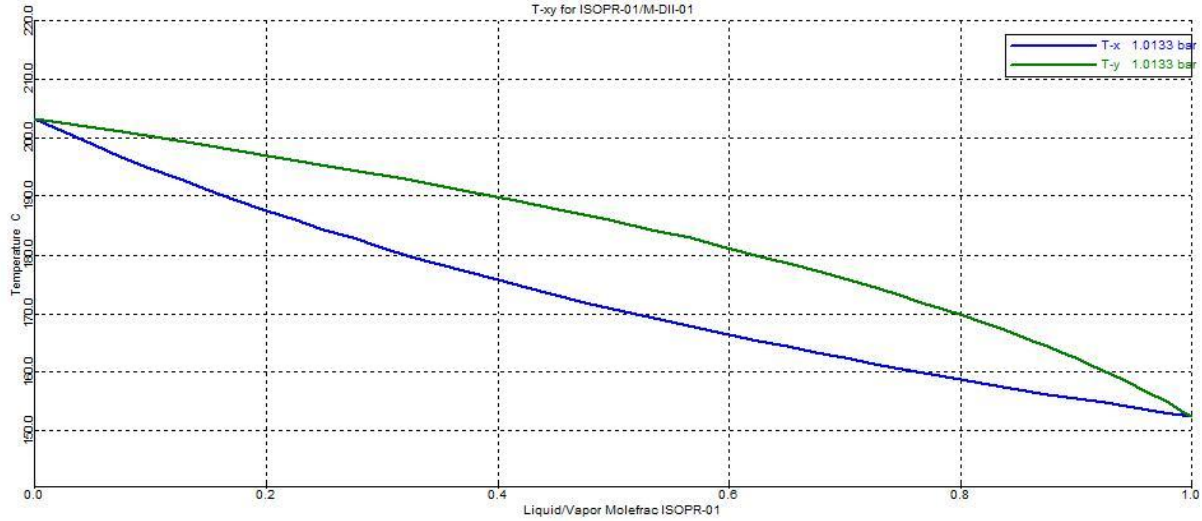


Fig 3.6 Txy for cumene-m-DIPB system

It can be inferred from plots Fig. 3.4 to 3.6 that separation would be easy and a distillation column with fewer trays and a smaller reflux ratio can be used. Azeotrope is not formed. Flash distillation should be tried as separation is easier.

3.4 FLASH DISTILLATION TANK DESIGN

Distillation is tried using flash tank as the cost of operation is very low. FLASH2 model is selected. SYSOP0 property method is selected, which works by ideal or Roult's law. Pressure of the flash tank is set as 1 bar. The input flow rate is same as mentioned in Table 3.2. The minimum boiling point in the mixture is that of benzene at 80.2 degree C at 1 atm and hence

a temperature of 85 to 97.5 is considered for flashing. The mole fractions of benzene and cumene in the bottom and top products are found out at various flashing temperatures and plotted in Fig. 3.7.

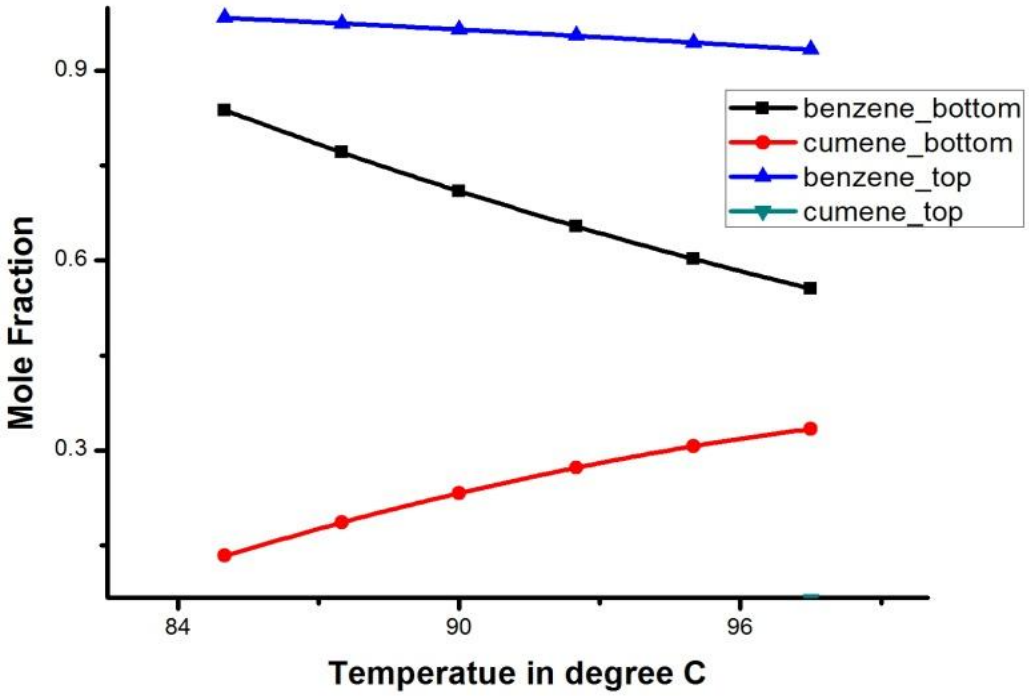


Fig 3.7 Temperature of flashing vs Mole fraction in top and bottom product of cumene and benzene

Assuming a product purity of 95% benzene in the top product the flashing temperature is identified to be 92.5 degree C. The flow rates of products from the flash tank are shown in Table 3.4.

Table 3.4 Flow rates of products from the flash tank

92.5 degree C	Benzene	Cumene	m-DIPB	p-DIPB
BOTTOM Product	18.951865	7.89384963	1.68473832	0.45287993
TOP product	5.39E+01	2.41615031	0.08526167	0.01712006

The flow rates of Table 3.4 act as a feed to the benzene column.

3.5 BENZENE DISTILLATION COLUMN DESIGN

3.5.1 DESIGN PROCEDURE

RADFRAC-1 is selected for designing the Benzene distillation column. SYSOP0 property method is selected and the flow rates from Table 3.4 are used. The pressure is kept fixed at 1.75 bar and the temperature is kept fixed at 90 degree Celsius. These two variables are obtained from the experimental data specified by Turton et al (2003). These temperature and pressure data have been used in the work by Luyben (2010). The variables that can be optimized are *reflux ratio, number of feed trays, feed tray location and distillate rate*. In the initial assumption the distillate rate is kept at half the value of the feed rate. A total condenser is used in the process and an equilibrium based approach is used.

3.5.2 REFLUX RATIO OPTIMIZATION

The number of trays (including boiler and condenser as a tray) is kept fixed at any value say 15. The feed tray is varied keeping the number of trays fixed. Now for each different ratio of number of trays to feed tray a series of reflux ratio starting from 0.1 is considered. The process is run and the mole fraction of benzene in the top product as well as the reboiler heat load data are used and a graph is plotted as shown in Fig 3.8. Reflux ratio is optimized by the variable mole fraction of benzene in the top product.

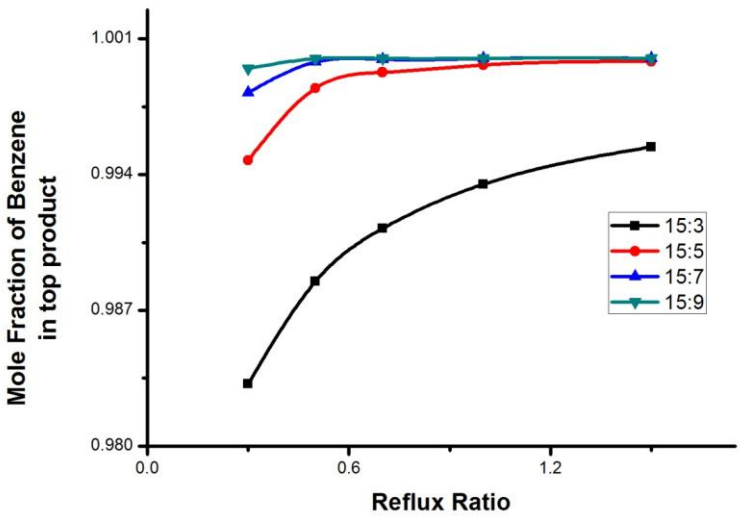


Fig 3.8 Reflux ratio vs Mole fraction of benzene in top product

An *optimum reflux ratio value of about 0.5* is identified from Fig 3.8. At higher values of feed tray location (close to reboiler) lesser reflux ratio is required. Note that condenser is considered as the first stage and the rebolier as the last.

3.5.3 FEED TRAY LOCATION OPTIMIZATION

The reflux ratio is kept fixed at 0.5 and the number of trays is kept fixed at 15. The position of the feed tray is varied and its affect on the reboiler heat load and the mole fraction of benzene in the top product is studied by plotting graphs in Fig.3.9 and 3.10.

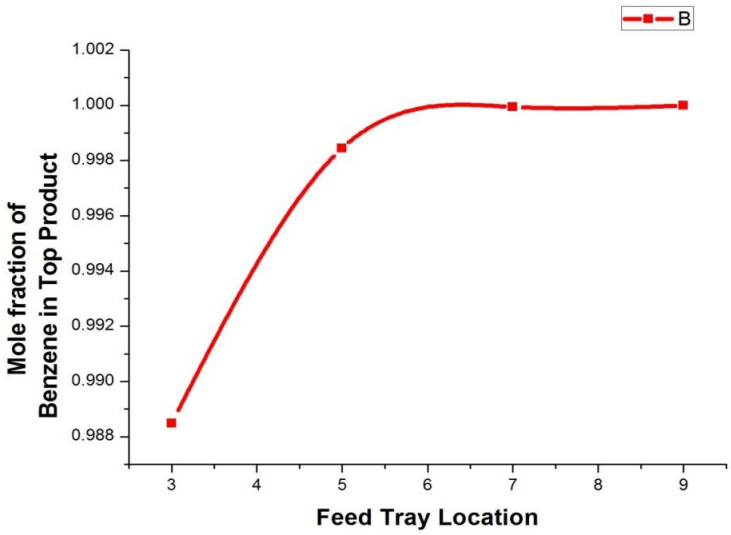


Fig 3.9 Feed tray location vs Mole fraction of benzene in top product

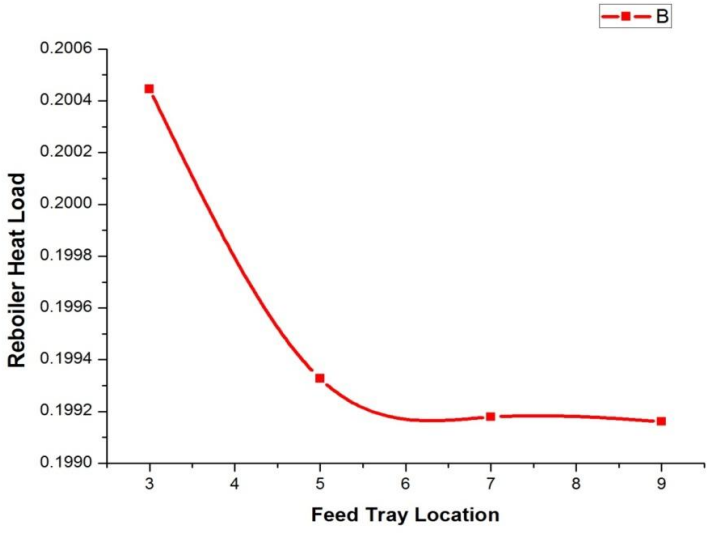


Fig 3.10 Feed tray location vs Reboiler heat load (Benzene Column)

From Fig. 3.9 and 3.10 it can be identified that after a certain optimum value of feed tray location is achieved there is hardly any change in the reboiler heat load and the concentration of benzene in the top product. *Ratio of 15 by 6 is identified as the optimum ratio*.

3.5.4 NUMBER OF TRAYS OPTIMIZATION

The ratio obtained above is kept constant and the number of trays is varied.

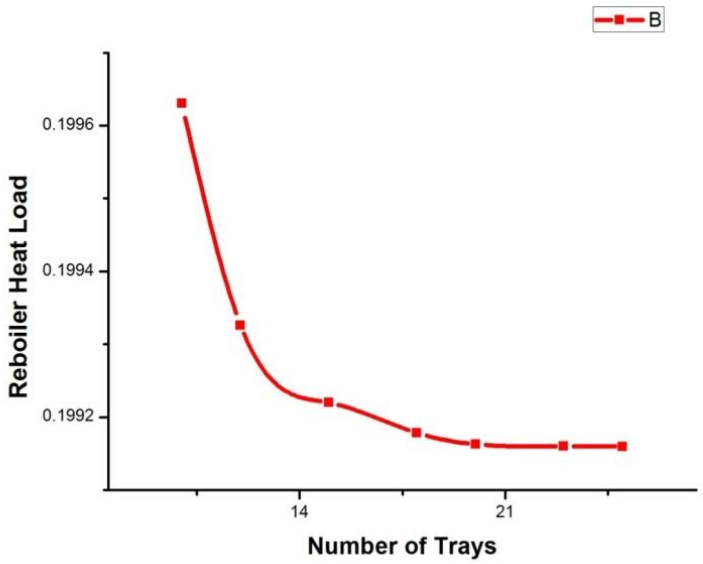


Fig 3.11 Number of trays vs Reboiler heat load (Benzene Column)

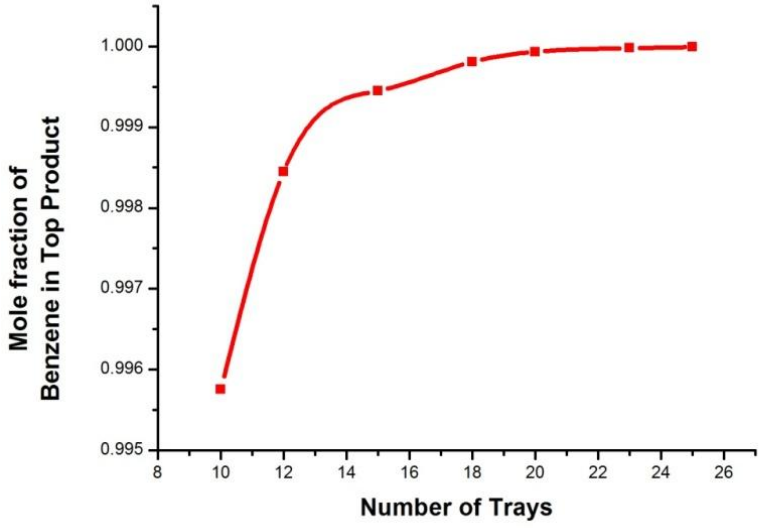


Fig 3.12 Number of trays vs Mole fraction of Benzene in top product

It can be identified from Fig. 3.11 and 3.12 that the product quality (mole fraction of benzene in top product) and the reboiler heat load donot vary significantly after an optimum number of trays is reached. *The optimum number of trays is obtained as 20.*

3.5.5 DISTILLATE RATE OPTIMIZATION

Distillate rate needs optimization as higher distillate rates can increase the quality and flow rate of top product but the reboiler heat load also significantly increases. Keeping distillate rates very high can improve the quality of top product but upto a certain limit. Very high distillate rates prevent proper separation. The mole fractions of cumene and benzene in the top and bottom products are plotted in Fig. 3.13.

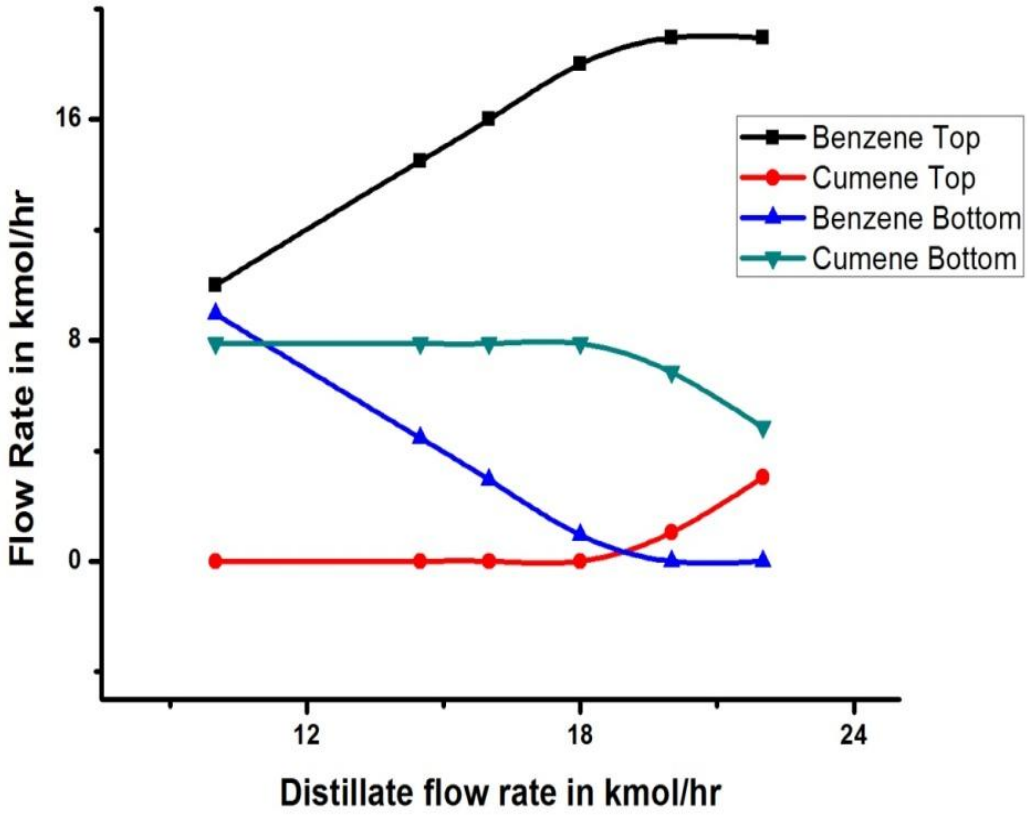


Fig. 3.13 Flow rate of components in top product and bottom product vs distillate rate (flow rates in kmol/hr)

Table 3.5 Product flow rate values at different distillate rates

Distillate flow rate kmol/hr	Benzene flow rate top product kmol/hr	Cumene flow rate top product kmol/hr	Benzene flow rate bottom product kmol/hr	Cumene flow rate bottom product kmol/hr
10	9.99929576	0.00070424	8.95256924	7.893145
14.4916664	14.49071	0.00095639	4.46115496	7.892893
16	15.9989608	0.00103922	2.95290423	7.89281
18	17.9988608	0.00113924	0.95300427	7.89271
20	18.9518649	1.04812842	8.41E-08	6.845721
22	1.90E+01	3.04806548	1.66E-08	4.845784

The quality of top product changes significantly in the 18 – 20 kmol/hr distillate flow rate region. The product quality initially increases as can be seen from Fig. 3.13 but after a certain value of distillate rate it doesn't rise. The Table 3.5 gives an idea about the flow rates of various components in top and bottom products on variation of distillate rate. The final optimized values for the benzene column are shown in Table 3.6.

Table 3.6 Final optimized values of benzene column

Number of Trays	20
Feed Tray Location	8
Reflux Ratio	0.5
Distillate Rate	19 kmol/hr
Temperature*	90 degree C
Pressure*	1.75 bar
* Literature Data	

3.6 CUMENE DISTILLATION COLUMN DESIGN

3.6.1 DESIGN PROCEDURE

RADFRAC-1 is selected for designing the cumene distillation column. SYSOP0 is selected and the bottom product flow rate values from the benzene column are the feed flow rate values to the cumene column. The pressure is kept fixed at 1 bar and the temperature is kept fixed at 164 degree Celsius. Higher temperature data gave iteration errors and hence all work is carried out at this temperature. The pressure data has been used in current research papers [Luyben, 2010]. Now in the cumene distillation column the variables that can be optimized are reflux ratio, number of feed trays, feed tray location and distillate rate. In the initial assumption the distillate rate is kept at half the value of the feed rate. A total condenser is used in the process and an equilibrium based approach is used. The bottom products from the cumene column are scaled up by a factor of 10 before optimization is started. The scaled up values are represented in Table 3.7 below.

Table 3.7 Flow rates of feed to cumene column after scale up

	Benzene	Cumene	m-DIPB	p-DIPB	Total
Original	2.97E-07	7.8457144	1.68473826	0.45287993	9.98
Scaled up (× 10)	2.97E-06	78.5	16.8	4.53	99.8

3.6.2 REFLUX RATIO OPTIMIZATION

The number of trays is fixed at any value say 15. The feed tray location is varied keeping the number of trays fixed. Now for each different ratio of number of trays to feed tray location a series of reflux ratio starting from 0.1 is considered. The process is run and the mole fraction of benzene in the top product as well as the reboiler heat load data are used and Fig. 3.14 is obtained by plotting.

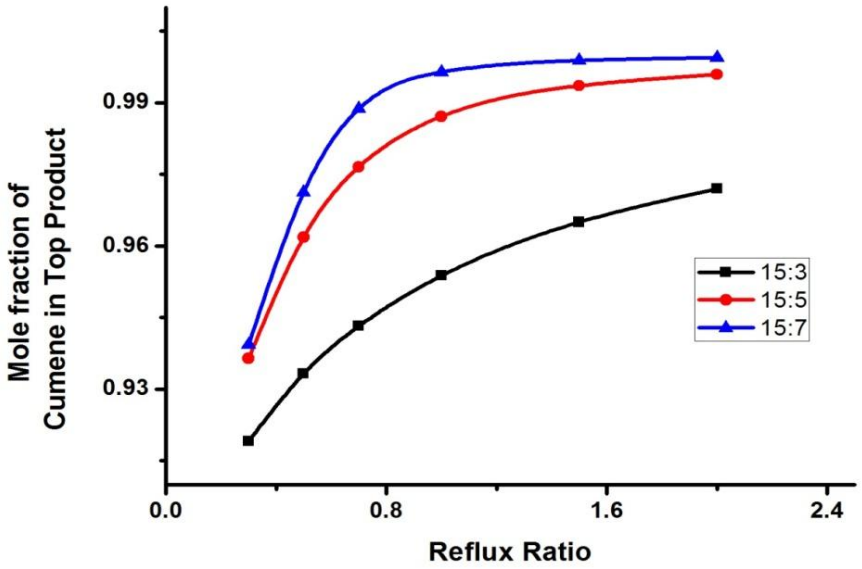


Fig 3.14 Reflux ratio vs Mole fraction of cumene in top product

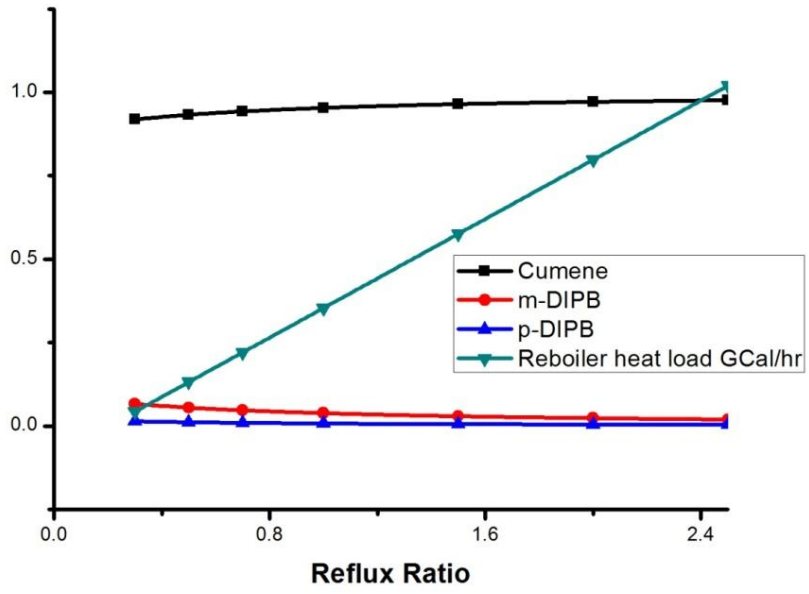


Fig 3.15 Reflux ratio vs mol fraction and reboiler heat load

Compared to benzene column the cumene column performs better at higher values of reflux ratio. It can be explained easily because the Txy diagrams for cumene-DIPB systems are thinner than Txy diagrams for Benzene-DIPB and hence separation is difficult. The plots

obtained in Fig. 3.14 and 3.15 are similar in structure to those for benzene. From the plots a optimum reflux ratio of 0.9 is identified.

3.6.3 FEED TRAY LOCATION OPTIMIZATION

A process similar to that described in 3.5.3 is followed.

Fig. 3.16 Feed tray location vs Mole fraction of cumene in top product

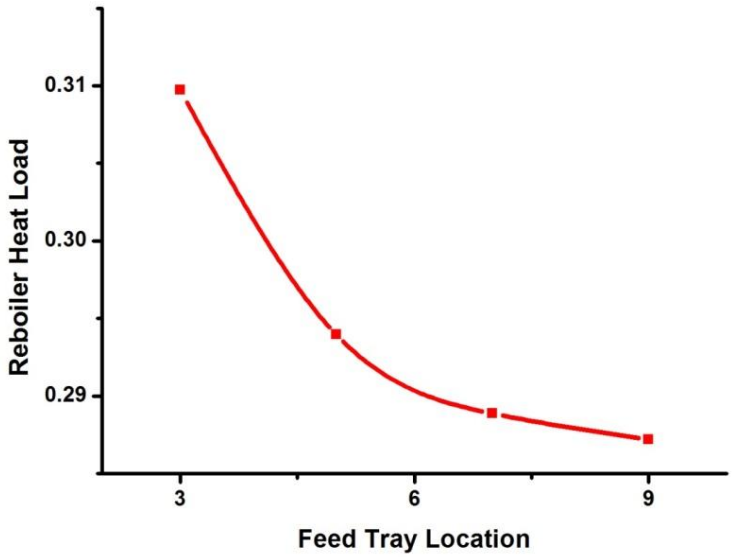


Fig 3.17 Feed tray location vs Reboiler heat load

It can be identified from Fig. 3.16 and 3.17 that the optimum number of trays: feed tray location is 15:7.5 or 2:1.

3.6.4 NUMBER OF TRAYS OPTIMIZATION

The all above parameters are kept fixed and the number of trays is varied keeping the ratio fixed.

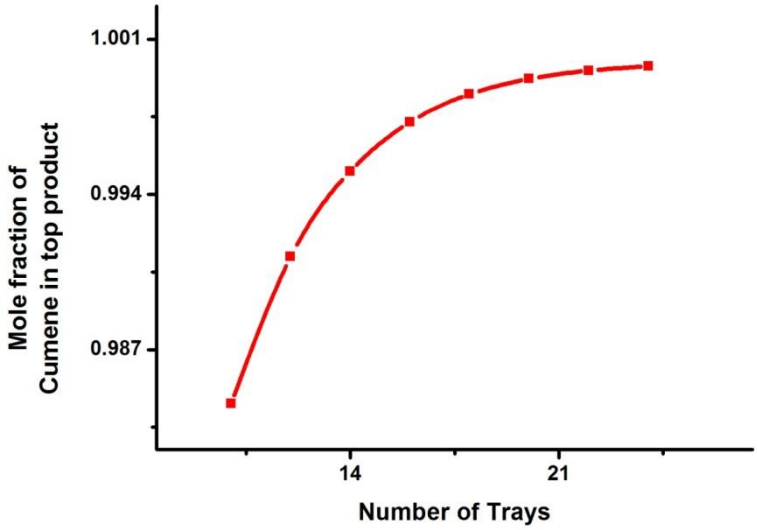


Fig 3.18 Number of trays vs mole fraction of cumene in top product

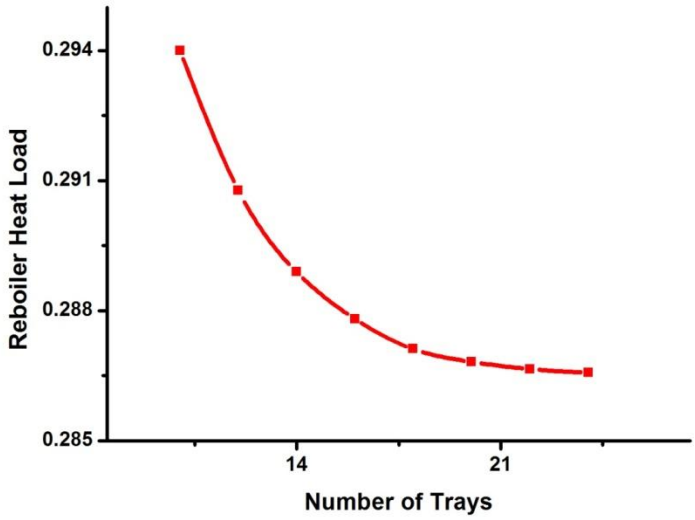


Fig. 3.19 Number of trays vs reboiler heat load

The optimum number of trays can be identified to be 20 from Fig. 3.18 and 3.19.

3.6.5 DISTILLATE RATE OPTIMIZATION

Now keeping other conditions fixed the distillate rate is varied.

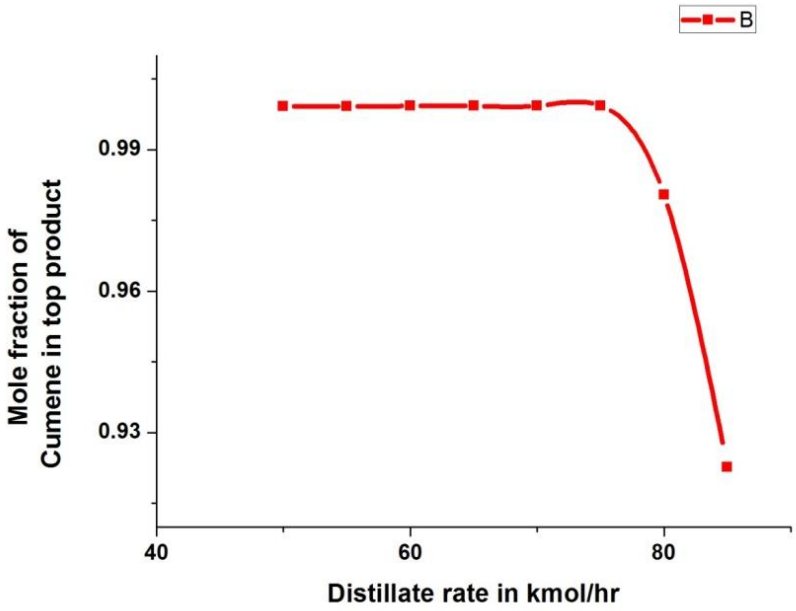


Fig 3.20 Distillate rate vs mole fraction of cumene in top product

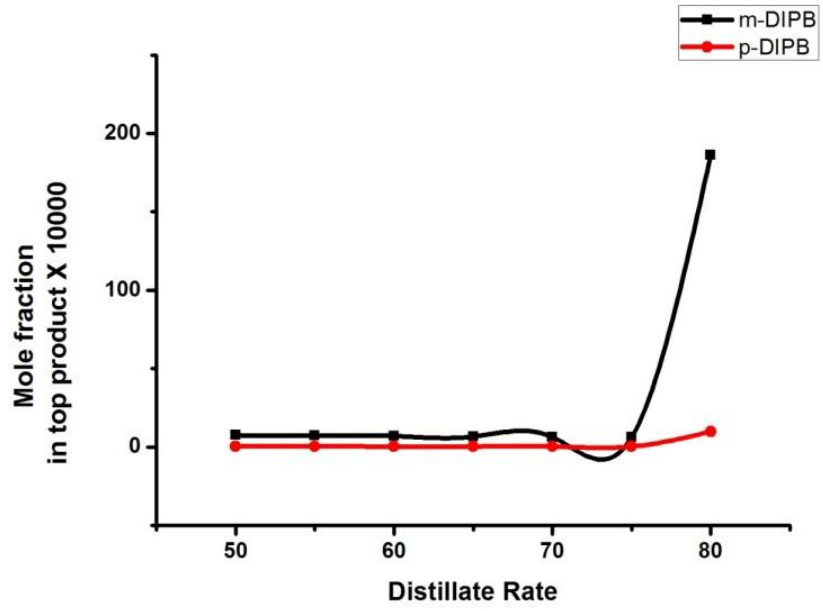


Fig 3.21 Distillate rate vs m-DIPB and p-DIPB mole fractions in top product

If heat of reboiler data which increases in a straight line has very less effect then the distillation rate can be safely optimized to be at 75 kmol/hr or 7.5 kmol/hr (without scaleup). The plot obtained in Fig. 3.20 and 3.21 are similar to those for benzene column. It can be

seen that the quality of the top product increases on increasing the distillate rate but upto a certain optimum distillate rate only.

3.7 RESULTS OF OPTIMIZATION

The results obtained in the current optimization project have been summarized below in the form of a brief flowsheet in Fig. 3.22.

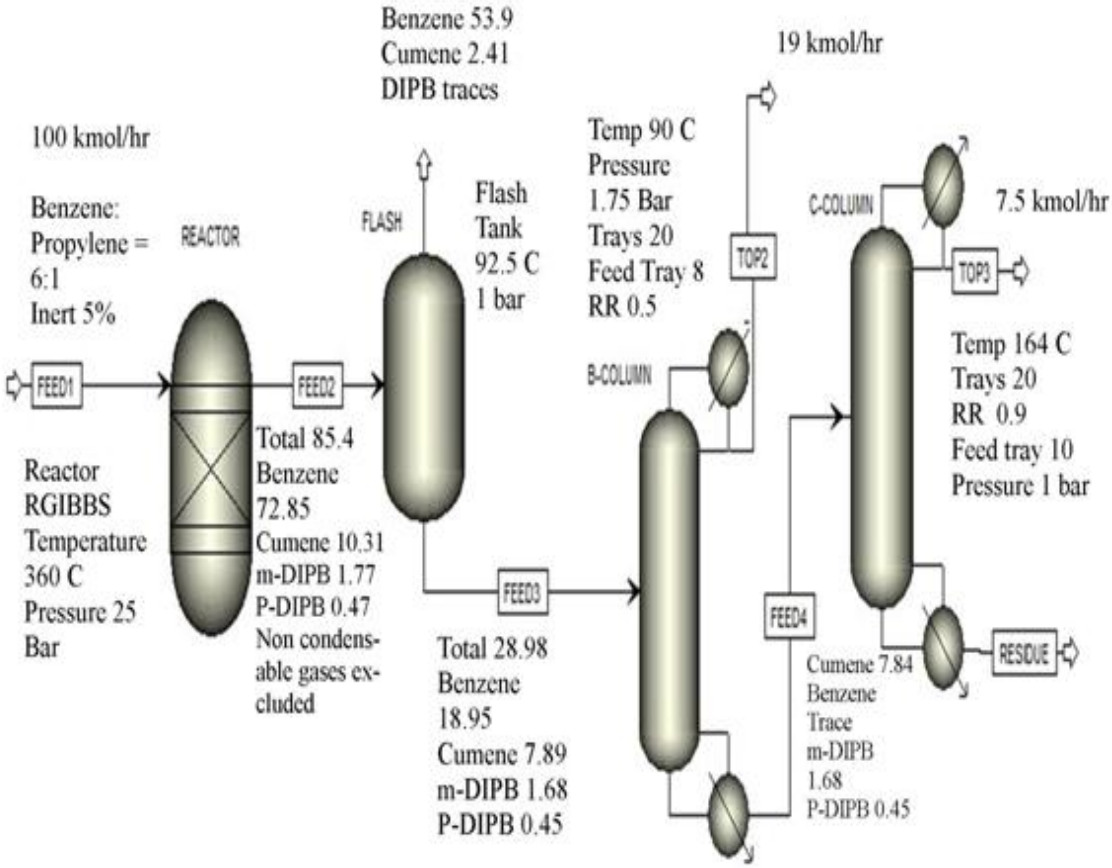


Fig 3.22 Flow rates and other parameters obtained by optimization.

CHAPTER 4

CONCLUSIONS

4. CONCLUSIONS

A step by step optimization procedure is followed in the present work. The basic components of a cumene plant are (1) Reactors and (2) Separators. Each unit is optimized by maximizing the quality of the desired product as well as its flow rate. This procedure is adapted from Douglas Doctrine (*Douglas Doctrine:* The costs of raw materials and products are usually much larger than the costs of energy or capital in a typical chemical process. Therefore the process must be designed (investing capital and paying for energy) so as to not waste feed stocks or lose products (particularly in the form of undesirable products) [Luyben, 2010]). After a unit is optimized, optimum flow rates are obtained. These flow rate values are used for optimizing the next unit.

The reactor system is optimized by an equilibrium based approach. The optimum values of temperature and feed concentrations are obtained as 360 degree C and 6:1 benzene: Propylene ratio respectively, by maximizing the selectivity towards cumene. The conversion of the limiting reagent is also maximized. The effect of presence of inert is also studied.

The separator system design begins with the plotting of VLE curves for possible mixtures. It can be concluded from the VLE plots that separation is easier for benzene-cumene-DIPB system. Flash distillation is tried before actual fractional distillation as the operating costs are very low. The optimum temperature for flashing is estimated. The distillation columns i.e. benzene column and cumene column depend on a large number of variables (high degree of freedom). Each variable is optimized by keeping the other values constant. After an optimum value of a variable is obtained the remaining variables are optimized using that data. The number of trays is found to be 20 for both while the feed tray location is 8 for benzene distillation column and 10 for cumene column. Reflux ratios are obtained as 0.5 and 0.9 respectively. The flashing temperature of the flash distillation tank is found to be 92.5 degree C. The flow rates and distillate rate data are shown in the optimised flow sheet given in the previous chapter.

Reactor and distillation column design revealed a lot of design considerations. For example in distillation column design if distillate rate is increased the product quality and the flow rate of the desired product increase but after a certain value (optimum value) the product quality and

flow rate reduce drastically. Similar findings were obtained while optimizing other units and they have been discussed briefly in the previous pages.

Again design solution cannot be considered absolute. For example if we decrease the reaction costs, the separation costs tend to increase. The design should not only take cost into consideration but also other factors such as safety, environmental impact, future needs etc.

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